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Isospin mixing in the vicinity of the $N = Z$ line

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We present the isospin- and angular-momentum-projected nuclear density functional theory (DFT) and its applications to the isospin-breaking corrections to the superallowed β-decay rates in the vicinity of the $N = Z$ line. A preliminary value obtained for the Cabbibo-Kobayashi-Maskawa matrix element, $|V_{ud}| = 0.97463(24)$, agrees well with the recent estimate by Towner and Hardy [Phys. Rev. C**77**, 025501 (2008)]. We also discuss new opportunities to study the symmetry energy by using the isospin-projected DFT.

1. Introduction

The isospin-symmetry violation in atomic nuclei is predominantly due to the Coulomb interaction that exerts long-range polarizations on neutron and proton states. To consistently take into account this polarization, one needs to employ huge configuration spaces. For that reason, an accurate description of isospin impurities in atomic nuclei, which is strongly motivated by the recent high-precision measurements of the $0^+ \to 0^+$ Fermi superallowed β-decay rates, is difficult to be obtained in shell-model approaches, and specific approximate methods are required.[1,2]

The long-range polarization effects can be included within the self-consistent mean-field (MF) or DFT approaches, which are practically the only microscopic frameworks available for heavy, open-shell nuclei with many valence particles. These approaches, however, apart from the *physical* contribution to the isospin mixing, mostly caused by the Coulomb field and, to a much lesser extent, by isospin-non-invariant components of the nucleon-nucleon force, also introduce the spurious isospin mixing due to the *spontaneous* isospin-symmetry breaking.[3,4,5]

Hereby, we present results on the isospin mixing and isospin symmetry-breaking corrections to the superallowed Fermi β-decay obtained by using the newly developed isospin- and angular-momentum-projected DFT approach without pairing.[6,7,8,9] The model employs symmetry-restoration techniques to remove the spurious isospin components and restore angular momentum symmetry, and

takes advantage of the natural ability of MF to describe self-consistently the subtle balance between the Coulomb force making proton and neutron wave functions different and the isoscalar part of the strong interaction producing the opposite effect.

The paper is organized as follows. In Sec. 2, we describe the main theoretical building blocks of the isospin- and angular-momentum-projected DFT. Section 3 presents some preliminary applications of the formalism to the isospin symmetry-breaking corrections to the Fermi superallowed β-decay matrix elements, whereas Sec. 4 discusses applications of the isospin-projected DFT to nuclear symmetry energy. The summary is contained in Sec. 5.

2. The projected DFT framework

The building block of the isospin-projected DFT is the Slater determinant, $|\Phi\rangle$, representing the self-consistent Skyrme-HF solution provided by the HF solver HFODD.[10] Self-consistency ensures that the balance between the long-range Coulomb force and short-range strong interaction, represented in our model by the Skyrme energy density functional (EDF), are properly taken into account. The unphysical isospin mixing is taken care of by the rediagonalization of the entire Hamiltonian in the good isospin basis, $|T, T_z\rangle$, as described in Refs.[8,9] This yields the eigenstates:

$$|n, T_z\rangle = \sum_{T \geq |T_z|} a^n_{T,T_z} |T, T_z\rangle \tag{1}$$

numbered by an index n. The so-called isospin-mixing coefficients (or, equivalently, isospin impurities) are defined for the $n-$th eigenstate as

$$\alpha^n_C = 1 - |a^n_{T,T_z}|^2_{\max}, \tag{2}$$

where $|a^n_{T,T_z}|^2_{\max}$ stands for the dominant amplitude in the wave function $|n, T_z\rangle$.

Within the isospin- and angular-momentum-projected DFT, we use the normalized basis of states $|I, M, K; T, T_z\rangle$ having both good angular momentum and good isospin.[11] Here, M and K denote the angular-momentum components along the laboratory and intrinsic z-axes, respectively. The K quantum number is not conserved. In order to avoid problems with overcompleteness of the basis, the K-mixing is performed by rediagonalizing the Hamiltonian in the so-called *collective space*, spanned for each I and T by the *natural states*, $|IM; TT_z\rangle^{(i)}$, as described in Refs.[10,12] Such a rediagonalization yields the eigenstates:

$$|n; IM; T_z\rangle = \sum_{i, T \geq |T_z|} a^{(n)}_{iIT} |IM; TT_z\rangle^{(i)}, \tag{3}$$

which are labeled by the index n and by the conserved quantum numbers I, M, and $T_z = (N - Z)/2$ [compare Eq. (1)].

The isospin projection does not produce singularities in energy kernels; hence, it can be safely used with all commonly used EDFs.[8] Coupling the isospin and

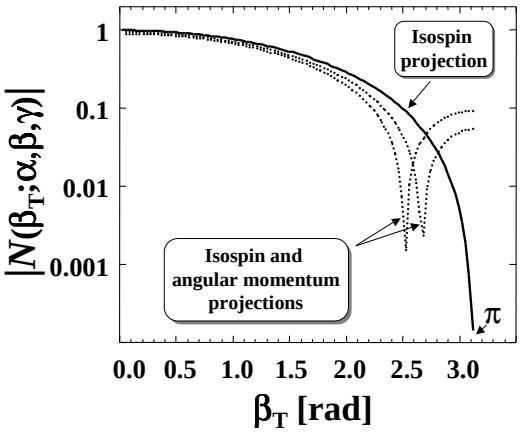

Fig. 1. The absolute values of the norm kernels, $|\mathcal{N}(\beta_T;\alpha,\beta,\gamma)| = |\langle\Phi|\hat{R}(\beta_T)\hat{R}(\alpha,\beta,\gamma)|\Phi\rangle|$, for a state in ^{14}N calculated with the SLy4 EDF, plotted versus the rotation angle in the isospace β_T. The solid curve, exhibiting the single singularity at $\beta_T = \pi$, corresponds to the pure isospin-projected DFT theory, which is regular for all Skyrme-type functionals.[8] The dotted lines correspond to two fixed sets of the Euler angles in space, with $\alpha = \gamma \approx 0.314$, and $\beta \approx 0.229$ (left curve) and $\beta \approx 1.414$ (right curve). The poles that appear inside the integration region, $0 < \beta_T < \pi$, give rise to singularities in the projected DFT approach.

angular-momentum projections, however, leads to singularities in both the norm (see Fig. 1) and energy kernels. This fact narrows the applicability of the model to Hamiltonian-driven EDFs which, for Skyrme-type functionals, leaves only one option: the SV parametrization.[13] The alternative would be to use an appropriate regularization scheme, which is currently under development.[14,15]

3. Isospin-mixing and isospin-breaking corrections to superallowed β-decay

Evaluation of α_C is a prerequisite to calculate isospin corrections to reaction and decay rates. As is well known,[17] isospin impurities are the largest in $N = Z$ nuclei, increase along the $N = Z$ line with increasing proton number, and are strongly quenched with increasing $|T_z| = |N - Z|/2$. Such characteristics were also early estimated based on the perturbation theory[18] or hydrodynamical model.[19] Quantitatively, after getting rid of the spurious mixing, which lowers the true α_C by as much as 30%,[7] the isospin impurity increases from a fraction of a percent in very light $N = Z$ nuclei to $\sim$0.9% in ^{40}Ca, and $\sim$6.0% in ^{100}Sn, as shown in Fig. 2. In the particular case of ^{80}Zr, the calculated impurity of 4.4% agrees well with the empirical value deduced from the giant dipole resonance γ-decay studies.[20] This makes us believe that our model is indeed capable of capturing essential physics associated with the isospin mixing. Unfortunately, current experimental errors are too large to discriminate between different parametrizations of the Skyrme functional. The

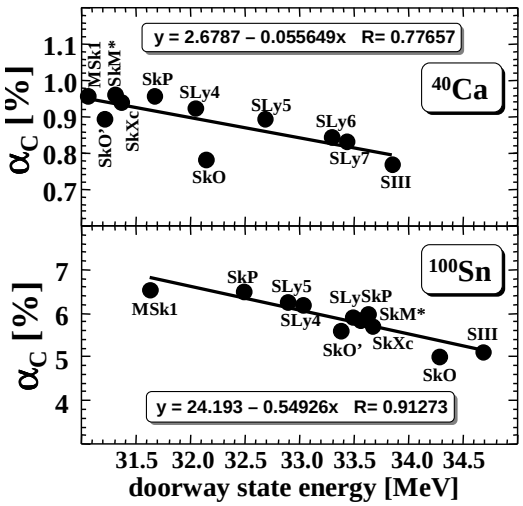

Fig. 2. Isospin impurities in the ground states of ^{40}Ca (upper panel) and ^{100}Sn (lower panel), plotted as functions of the excitation energy of the doorway state for a set of commonly used Skyrme EDFs.[16] Results of the linear fits and the corresponding regression coefficients, R, are also shown.

variations between EDFs in Fig. 2 result in $\sim$10% uncertainty in calculated values of α_C.

The magnitude of theoretical α_C is quite well correlated with the excitation energy, $E_{T=1}$, of the $T = 1$ doorway state, see Fig. 2. However, in order to make a precise determination of $E_{T=1}$, spectroscopic quality EDFs are needed, and this is not yet the case.[21] This explains why the values of α_C do not correlate well with basic EDF characteristics, including the isovector and isoscalar effective mass, symmetry energy, binding energy per particle, and incompressibility (see discussion in Ref.[9]).

Increasing demand on precise values of isospin impurities has been stimulated by the recent high-precision measurements of superallowed β-decay rates.[26,2] A reliable determination of the corresponding isospin-breaking correction, δ_C, requires the isospin- and angular-momentum-projected DFT.[9]. This correction is obtained by calculating the $0^+ \to 0^+$ Fermi matrix element of the isospin raising/lowering operator $\hat{T}_\pm$ between the ground state (g.s.) of the even-even nucleus $|I = 0, T \approx 1, T_z = \pm 1\rangle$ and its isospin-analogue partner in the $N = Z$ odd-odd nucleus, $|I = 0, T \approx 1, T_z = 0\rangle$:

$$|\langle I = 0, T \approx 1, T_z = \pm 1|\hat{T}_\pm|I = 0, T \approx 1, T_z = 0\rangle|^2 \equiv 2(1 - \delta_C). \tag{4}$$

To determine the $|I = 0, T \approx 1, T_z = 0\rangle$ state in the odd-odd $N = Z$ nucleus, we first compute the so-called antialigned g.s. configuration, $|\bar{\nu} \otimes \pi\rangle$ (or $|\nu \otimes \bar{\pi}\rangle$), by placing the odd neutron and the odd proton in the lowest available time-reversed (or signature-reversed) HF orbits. Then, to correct for the fact that the antialigned

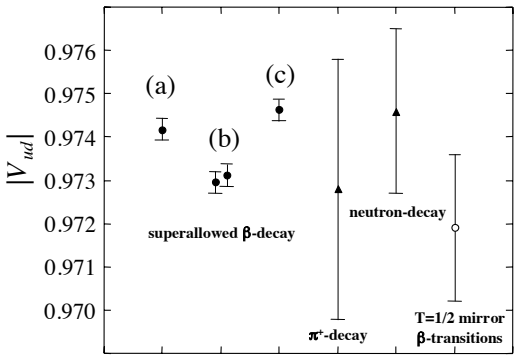

Fig. 3. Values of $|V_{ud}|$ deduced from the superallowed β-decay (full circles) for three different sets of the δ_C corrections calculated in: Ref.[2] (a); Ref.[22] with NL3 and DD-ME2 Lagrangians (b); and in the present work (c). Triangles mark values of $|V_{ud}|$ obtained from the pion-decay[23] and neutron-decay[24] studies, respectively. The open circle shows the value deduced from the β-transitions in $T = 1/2$ mirror nuclei.[25]

configurations manifestly break the isospin symmetry,[8] that is, $|\bar{\nu} \otimes \pi\rangle \approx \frac{1}{\sqrt{2}}(|T = 0\rangle + |T = 1\rangle)$, we apply the isospin and angular-momentum projections to create the basis $|I, M, K, T, T_z = 0\rangle$, in which the total Hamiltonian is rediagonalized (see Sec. 2). A similar scheme is used to compute the $|I = 0, T \approx 1, T_z = \pm 1\rangle$ states in the even-even nuclei.

Our studies indicate[9] that to obtain a fair estimate of δ_C for $A < 40$ and $A > 40$ nuclei, one needs to use large harmonic oscillator bases consisting of at least $N = 10$ and 12 full shells, respectively. Even then, the results are subject to systematic errors due to the basis cut-off, which can be estimated to be $\sim$10%. Despite the fact that not all $N = 12$ calculations in heavy ($A > 40$) nuclei have yet been completed, and that owing to the shape-coexistence effects, there are still some ambiguities concerning the global minima, our preliminary results point to encouraging conclusions. Namely, the mean value of the structure-independent statistical-rate function $\bar{\mathcal{F}}t$,[26] obtained for 12 out of 13 transitions known empirically with high precision (excluding the ^{38}K$\rightarrow^{38}$Ar case), equals $\bar{\mathcal{F}}t = 3069.4(10)$, which gives the value of the CKM matrix element equal to $|V_{ud}| = 0.97463(24)$. These values match well those obtained by Towner and Hardy in their recent compilation[2] (see Fig. 3). Because of a poor spectroscopic quality of the SV parameterization, the confidence level[27] of our results is poor. Nevertheless, it should be stressed that our method is quantum-mechanically consistent (see discussion in Refs.[28,29]) and contains no adjustable free parameters.

4. Symmetry energy

The spontaneous violation of isospin symmetry in all but isoscalar MF configurations of $N = Z$ nuclei offers a way to study the nuclear symmetry energy. The idea,

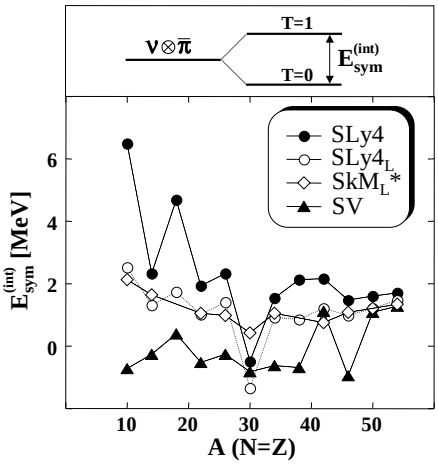

Fig. 4. Top: schematic illustration of the isospin-symmetry-breaking mechanism in MF of odd-odd $N = Z$ nuclei. Bottom: $E_{\rm sym}^{\rm (int)}$ in odd-odd $N = Z$ nuclei calculated with SLy4, SV, SLy4$_L$, and SkM$_L^*$ EDFs. See text for details.

which is schematically sketched in the upper portion of Fig. 4, invokes the mixed-symmetry antialigned $|\bar{\nu} \otimes \pi\rangle$ (or $|\nu \otimes \bar{\pi}\rangle$) configuration in an odd-odd $N = Z$ nucleus. By applying the isospin projection to the HF state $|\bar{\nu} \otimes \pi\rangle$, one decomposes it into the isoscalar $T = 0$ and isovector $T = 1$ parts. As argued below, the magnitude of the splitting, $E_{\rm sym}^{\rm (int)}$, depends on the isovector channel of a given EDF, i.e., its symmetry energy.

For the Skyrme-type EDFs, the symmetry energy in the nuclear matter limit can be decomposed as:[30]

$$a_{\rm sym} = \frac{1}{8}\varepsilon_{FG}\left(\frac{m}{m_0^\star}\right) + \left[\left(\frac{3\pi^2}{2}\right)^{2/3} C_1^\tau \rho^{5/3} + C_1^\rho \rho\right] \equiv a_{\rm sym}^{\rm (kin)} + a_{\rm sym}^{\rm (int)}. \qquad (5)$$

The first term in Eq. (5) is associated with the isoscalar part of the nucleon-nucleon interaction and primarily depends on the mean single-particle level spacing at the Fermi energy. This term is scaled by the inverse isoscalar effective mass. The second (interaction) term, is related to the isovector part of the Skyrme-EDF: $\delta\mathcal{H}_{t=1} = C_1^\rho \rho_1^2 + C_1^\tau \rho_1 \tau_1$ (for definitions, see Ref.[16] and references quoted therein).

The value of $E_{\rm sym}^{\rm (int)}$ appears to be mainly sensitive to the interaction term, which is illustrated in Fig. 4. Indeed, despite the fact that SLy4 and SV EDFs have similar values of $a_{\rm sym}$ (equal to 32 MeV and 32.8 MeV, respectively), the corresponding energy splittings $E_{\rm sym}^{\rm (int)}$ differ substantially. The reduced values of $|E_{\rm sym}^{\rm (int)}|$ in SV are due to its small value of $a_{\rm sym}^{\rm (int)} = 1.4\,{\rm MeV}$,[a] which is an order of magnitude smaller

[a] This small value shows how unphysical are the consequences of the saturation mechanism built into SV through the strong momentum dependence and results in an unphysically low isoscalar

than the corresponding SLy4 value: $a_{\rm sym}^{\rm (int)} = 14.4\,{\rm MeV}$.

An interesting aspect of our analysis of $E_{\rm sym}^{\rm (int)}$ relates to its dependence on the time-odd terms, which are poorly constrained for Skyrme EDFs. To quantify this dependence, we have performed calculations by using the SLy4$_L$ and SkM$^*_L$ functionals, which have the spin coupling constants adjusted to the Landau parameters.[31,32] These EDFs have different values of $a_{\rm sym}$ but the same $a_{\rm sym}^{\rm (int)} = 14.4\,{\rm MeV}$. The similarity of the calculated energy splittings shown in Fig. 4 confirms that this quantity primarily depends on the isovector terms of the functional. Moreover, its significant dependence on the time-odd terms opens up new options for adjusting the corresponding coupling constants to experimental data. This will certainly require the simultaneous restoration of isospin and angular-momentum symmetries, as presented in this study.

5. Summary

In summary, the isospin- and angular-momentum-projected DFT calculations have been performed to estimate the isospin-breaking corrections to $0^+ \to 0^+$ Fermi superallowed β-decays. Preliminary results for the average value of the nucleus-independent $\bar{\mathcal{F}}t = 3069.4(10)$ and the amplitude $|V_{ud}| = 0.97463(24)$ were found to be consistent with the recent estimates by Towner and Hardy,[2] notwithstanding a low spectroscopic quality of the Skyrme EDF SV used.

Applicability of the isospin-projected DFT to analyze the nuclear symmetry energy has also been discussed. It has been demonstrated that the isospin projection offers a rather unique opportunity to study the interaction part of the symmetry energy in the odd-odd $N = Z$ nuclei and that this quantity is influenced by time-odd fields of the energy density functional.

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